

1-methoxypropan-2-yl 2-methylpropanoate

5436-79-3 | DTXSID40281472

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.21×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.91×10^{-1}

Confidence level: 8.54×10^{-1}

Nearest Neighbors from the Training Set

Image not found

2-Ethoxyethyl isobutyrate

Measured: 1.35×10^{-11}

Predicted: 1.28×10^{-11}

Image not found

Ethyl 3-ethoxypropionate

Measured: 2.29×10^{-11}

Predicted: 1.63×10^{-11}

Image not found

Butyl butyrate

Measured: 1.06×10^{-11}

Predicted: 1.06×10^{-11}

Image not found

Butanoic acid, propyl ester

Measured: 7.41×10^{-12}

Predicted: 6.98×10^{-12}

Image not found

Pentyl acetate

Measured: 7.55×10^{-12}

Predicted: 6.38×10^{-12}